

# The role of the initial state in the collapse of a Bose condensed gas

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The stability of a Bose condensed gas with a negative scattering length is studied with regard to the role played by the initial state. A trapped ideal gas ground state is shown to be unstable when the Gross Pitaevskii equation still predicts the existence of a stable state. A possible relation to a recent experimental study of the critical conditions for stability or collapse of a Bose Einstein condensate [J. L. Roberts et al., Phys. Rev. Lett. **86**, 4211 (2001)] is discussed.

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The possibility of manipulating interatomic forces using magnetic field tunable Feshbach resonances [1], has provided new opportunities for the study of collision phenomena in ultra cold gases. Recent experiments with  $^{85}\text{Rb}$  [2] have shown how one can tune the two body interaction, in a condensate from strongly repulsive to attractive over a wide range of different  $s$  wave scattering lengths. This makes possible the study of non equilibrium phenomena under a variety of controlled initial conditions. One of the most striking experiments of this type is that in which a condensate, first formed with repulsive forces, is switched to the attractive case, and collapses. In an idealized sense collapse means an unrestricted contraction of a gas within a finite amount of time. As shown by Pitaevskii [3], the time dependent Gross Pitaevskii equation (GPE) predicts this remarkable phenomenon for a trapped Bose condensed gas with a negative scattering length in a harmonic trap as soon as certain conditions, on the interaction strength, and the initial condensate wave function, are fulfilled.

Very recently, the control of the interatomic force in  $^{85}\text{Rb}$  [4] has allowed an experimental determination of the critical conditions for the stability, with respect to collapse, of a condensate. In the course of these experiments, the interatomic force of the gas was tuned towards specific negative  $s$  wave scattering lengths by means of magnetic fields, using a Feshbach resonance. Since the initial scattering length was chosen to be negligibly small, from the point of view of the GPE the prepared initial state can be interpreted as an ideal gas condensate wave function.

Since their first observation in experiments with  $^7\text{Li}$  [5], Bose condensed gases with a negative scattering length have been studied by numerous authors. Most of this work has used the GPE and focused on the stability conditions for a ground state solution (see, e.g., [6] and references therein) or condensate formation [7]. The experimental results in Ref. [4] indicate, however, that as soon

as the condensate becomes unstable the GPE alone is not suitable for the description of the dynamics of the collapse. In particular the observed substantial loss of condensate atoms contradicts the number conservation inherent in the GPE. This failure can be expected because the collision term of the GPE does not account for collisional losses of condensate atoms due to non forward scattering [8], which should become relevant for the rapid dynamics occurring during the collapse.

More interestingly the gas was seen to be unstable even under conditions, where the GPE predicts the existence of a stable ground state. To clarify this aspect of the observations we have studied the stability of a Bose condensed gas with a negative scattering length using the GPE, taking into account the role of the initial state, prepared in the experiment in Ref. [4]. We show that this initial ideal gas state leads to collapse condition that is different from that for the existence of a ground state of the condensate.

Throughout this article the  $s$  wave scattering length of the interatomic force,  $a_0$ , is assumed to be negative. For a Bose condensed gas in a spherical trap, with the harmonic potential  $V_{\text{trap}} = m\omega_{\text{ho}}^2 r^2/2$ , the natural units of time and length are the inverse trap frequency  $\omega_{\text{ho}}^{-1}$  and the harmonic oscillator length  $a_{\text{ho}} = \sqrt{\hbar/m\omega_{\text{ho}}}$ , respectively. Expressed through these units the GPE for an interacting Bose gas, consisting of  $N$  atoms, assumes the well known form [6]

$$i\frac{\partial}{\partial t}\psi = -\frac{1}{2}\Delta\psi + \frac{1}{2}r^2\psi - 4\pi k|\psi|^2\psi. \quad (1)$$

Here the condensate wave function  $\psi$  is normalized to unity,  $k$  is given by  $N|a_0|/a_{\text{ho}}$  and the corresponding unit of the energy is then  $N\hbar^2/ma_{\text{ho}}^2$ . Equation (1) shows that  $k$  is the only free adjustable parameter of the GPE for a spherical trap.

On first sight, the form of Eq. (1) might suggest that the critical conditions for collapse are governed solely by the parameter  $k$ . With respect to the existence of a stable ground state of a condensate this is true. In fact, the theoretical studies in Ref. [9,10] confirm the condition for stability

$$k < k_{\text{cr}} = 0.575. \quad (2)$$

When the initial condensate wave function deviates from the ground state, however, a collapse can occur even if the actual parameter  $k$  is well below the above standard value.

As proposed by Pitaevskii [3] the conditions for stability or collapse can be visualized by means of two fundamental estimates provided by the GPE. The first one is

the uncertainty relation between the mean square of the radius of a condensate,  $\langle r^2 \rangle = \int d\mathbf{r} r^2 |\psi|^2$ , and its kinetic energy,  $T = \int d\mathbf{r} |\nabla \psi|^2/2$ , which reads

$$\langle r^2 \rangle T \geq 9/8, \quad (3)$$

where the choice of units corresponds to Eq. (1). It is worth noting that once  $\langle r^2 \rangle$  vanishes the condensate wave function has collapsed. The kinetic energy then becomes infinite. The second estimate consists in an inequality between the mean field energy,  $E_{\text{mf}} = -4\pi k \int d\mathbf{r} |\psi|^4/2$ , and the kinetic energy,

$$\int d\mathbf{r} |\psi|^4/2 \leq \beta T^{3/2}, \quad (4)$$

where  $\beta = 0.0575$  is a universal constant. Equations (3) and (4) are preserved for all times by the GPE.

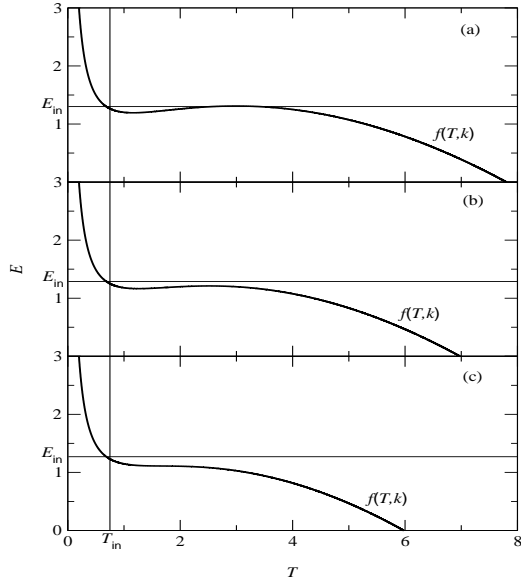


FIG. 1. Lower estimate for the total energy  $E$  as a function of the kinetic energy  $T$  for three different parameters of the interatomic force: (a)  $k = 0.5$ , (b)  $k = 0.53$  and (c)  $k = 0.575$ . The horizontal lines indicate the total energy for an initial ideal gas ground state condensate wave function. The vertical line indicates the initial kinetic energy of the Bose condensed gas. The energies are given in units of  $N\hbar^2/ma_{\text{ho}}^2$ . The accessible points  $(T, E)$  are above the curve  $f(T, k)$ .

As an additional constant of motion, the total energy,

$$E = T + V + E_{\text{mf}}, \quad (5)$$

contains the kinetic and the mean field part as well as the trap energy  $V = \int d\mathbf{r} V_{\text{trap}} |\psi|^2$ . In the spherical case

the mean square of the radius of a condensate and the trap energy are related through

$$V = \langle r^2 \rangle/2. \quad (6)$$

The inequality given by Eq. (3) then provides an estimate for the trap energy Eq. (6) through the kinetic energy. In addition, according to Eq. (4), the mean field contribution to the total energy Eq. (5) can be estimated in terms of  $T$ . This in turn implies the general relation

$$E \geq T + \frac{9}{16} T^{-1} - 4\pi\beta k T^{3/2} \equiv f(T, k), \quad (7)$$

which is valid for all times.

In Fig. 1 the lower bound Eq. (7) is illustrated for the parameters  $k = 0.5$  (Fig. 1a),  $k = 0.53$  (Fig. 1b) and  $k = 0.575$  (Fig. 1c) and an initial ideal gas ground state. For this Gaussian initial condensate wave function the total energy and the initial kinetic energy are given by  $E = E_{\text{in}} = 3/2 - k/\sqrt{2\pi}$  and  $T_{\text{in}} = 3/4$ , respectively. In Fig. 1a the function  $f(T, k)$  exhibits a local minimum which encloses the point  $(T_{\text{in}}, E)$ . As the total energy is a constant of motion and  $T(t)$  varies continuously in time the kinetic energy is caught in the valley for all times. As pointed out by Pitaevskii [3], the inequality given by Eq. (3) then predicts the mean square of the radius of the condensate to be positive, i.e.  $\langle r^2 \rangle \geq 9/8T > 0$ , and a total collapse, i.e.  $\langle r^2 \rangle = 0$ , can never occur. As can be seen in Fig. 1c, very close to the standard critical interaction strength Eq. (2) the function  $f(T, k)$  becomes monotonous. Hence, a ground state of the GPE ceases to exist as soon as the local minimum of  $f(T, k)$  vanishes.

In Fig. 1b, however, the total energy is above the local maximum of  $f(T, k)$  and at least the lower bound in Eq. (7) allows the kinetic energy to access arbitrarily high values. In this case a total collapse of the condensate wave function cannot be excluded by the inequality Eq. (3).

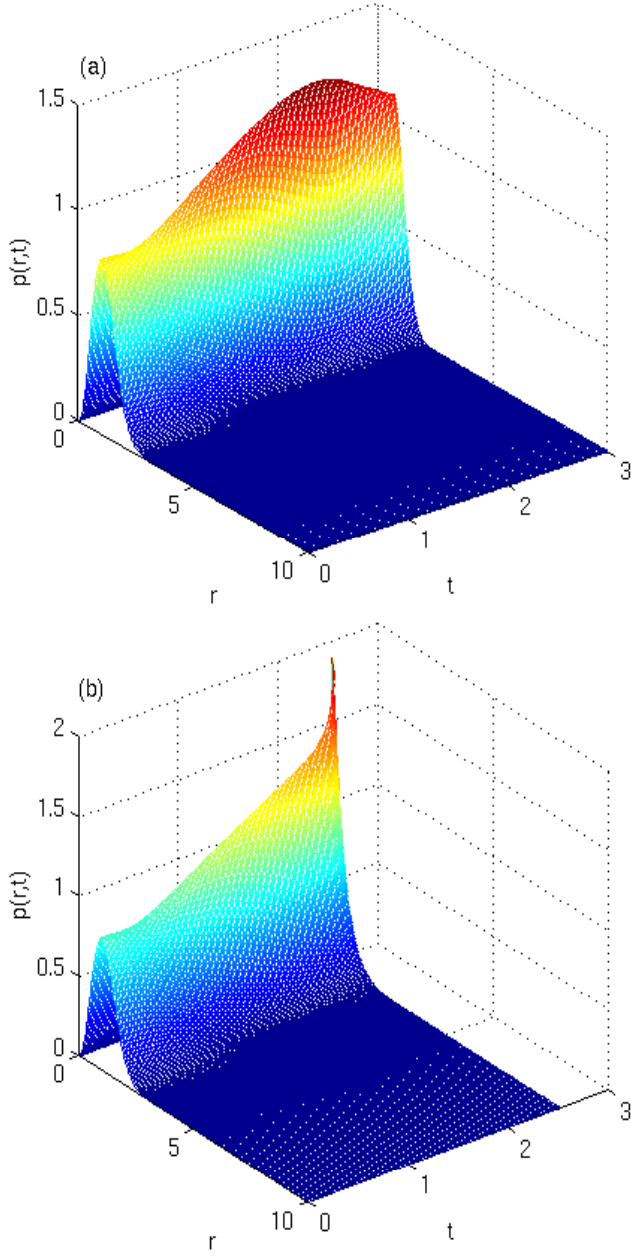


FIG. 2. Numerical solutions of the time dependent Gross Pitaevskii equation for a spherical trap with an initial ideal gas ground state condensate wave function and different parameters of the interatomic force: (a)  $k = 0.52$  and (b)  $k = 0.53$ . The graphs show the radial density  $p(r,t) = 4\pi r^2 |\psi(r,t)|^2$  as a function of the radius  $r$  and the time  $t$ . The time and the radius are given in units of the inverse trap frequency  $\omega_{ho}^{-1}$  and the harmonic oscillator length  $a_{ho} = \sqrt{\hbar/m\omega_{ho}}$ , respectively. The radial density is normalized to unity.

To clarify this situation, Fig. 2 shows the results of numerical simulations of the GPE in Eq. (1) for  $k = 0.52$  (Fig. 2a) and  $k = 0.53$  (Fig. 2b), with an initial ideal gas ground state condensate wave function. In Fig. 2a,

the simulation predicts the condensate to be stable with respect to collapse within the considered period of time. For the present parameter  $k = 0.52$  the total energy is already slightly above the local maximum of the function  $f(T,k)$  and a rigorous assertion concerning stability or collapse cannot be obtained directly from Pitaevskii's estimate.

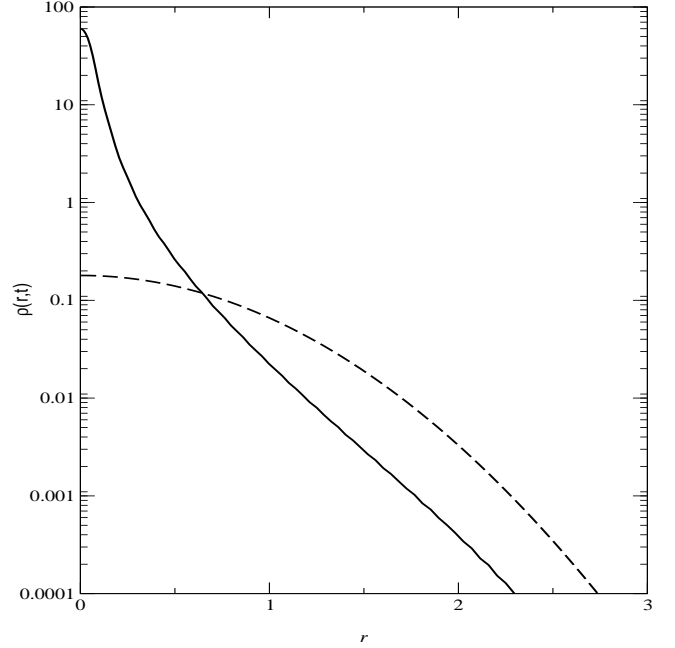


FIG. 3. Comparison of the spatial condensate density  $\rho(r,t) = |\psi(r,t)|^2$  at time  $t = 2.52 \omega_{ho}^{-1}$ , close to the collapse, (solid line) with the initial Gaussian density (dashed line) for  $k = 0.53$ . The unit of the radius  $r$  is chosen as in Fig. 2. The normalized densities ( $\int dr \rho(r,t) = 1$ ) are shown on a logarithmic scale.

In Fig. 2b, however, the condensate wave function exhibits a collapse although the actual parameter of the interatomic force of  $k = 0.53$  is still sufficiently weak for a stable ground state of the GPE to exist. To visualize the contraction of the condensate wave function, in Fig. 3 a typical density  $|\psi(r,t)|^2$ , close to the time of the collapse, is compared with the initial Gaussian density. The corresponding wave function is obtained from the simulation in Fig. 2b. As can be seen on the logarithmic scale, the predicted condensate density, close to the collapse, deviates from a Gaussian and exhibits a sharp peak at its center.

The GPE thus predicts the preparation of an initial ideal gas ground state condensate wave function to lead to a pronounced reduction of the critical parameter of the interatomic force to

$$k_{cr} \lesssim 0.53 \quad (8)$$

in comparison with the standard critical value for the existence of a stable ground state. This critical value for

an initial ideal gas ground state has been reported also in Ref. [10] as an intermediate result in the numerical study of stable ground states of the GPE. A numerical simulation alone, however, cannot predict stability of a condensate on arbitrarily long time scales. The required lower estimate of  $k_{\text{cr}}$  is thus provided by the analysis illustrated in Fig. 1 and yields

$$k_{\text{cr}} > 0.5. \quad (9)$$

The sharply defined critical parameter of

$$k_{\text{cr}} = 0.461 \pm 0.012 \pm 0.054, \quad (10)$$

reported in Ref. [4], is indeed significantly smaller than the predicted standard value for the existence of a stable ground state in Eq. (2). This corroborates the predictions of the GPE in view of the destabilizing role of the particular initial state that was prepared in the experiment. Equations (8) and (9), however, are not strictly valid in the experimental case because the magnetic field was ramped linearly to its final value rather than abruptly. Interestingly, though, our result obtained from the GPE agrees with the observations within the experimental upper limit for  $k_{\text{cr}}$ .

The analysis of stability or collapse of a dilute Bose condensed gas with a negative scattering length, performed in this work, can be applied to arbitrary initial condensate wave functions and trap geometries. The optimal estimate from Eq. (7) is obtained for a spherical trap. Related experiments with more general initial states should be feasible with the method described in Refs. [2,4] and could provide a further understanding of the range of validity of the GPE in non equilibrium situations.

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